Generalization of SGIP Surface Tension Force Model in Three-Dimensional Flows and Compare to Other Models in Interfacial Flows

Afshin Ahmadi Nadooshan, and Ebrahim Shirani

Abstract—In this paper, the two-dimensional stagger grid interface pressure (SGIP) model has been generalized and presented into three-dimensional form. For this purpose, various models of surface tension force for interfacial flows have been investigated and compared with each other. The VOF method has been used for tracking the interface. To show the ability of the SGIP model for three-dimensional flows in comparison with other models, pressure contours, maximum spurious velocities, norm spurious flow velocities and pressure jump error for motionless drop of liquid and bubble of gas are calculated using different models. It has been pointed out that SGIP model in comparison with the CSF, CSS and PCIL models produces the least maximum and norm spurious velocities. Additionally, the new model produces more accurate results in calculating the pressure jumps across the interface for motionless drop of liquid and bubble of gas which is generated in surface tension force.

Keywords—Volume-of-Fluid; SGIP model; CSS model; CSF model; PCIL model; surface tension force; spurious currents.

I. INTRODUCTION

ONE of the important subjects that have been considered by fluid mechanics researchers is studying and pondering the interfacial flows. Different numerical methods are employed and developed for simulating such flows. The numerical methods can be divided into two groups depending on the type of grids used: fixed grid or moving grid. For the first group, the interface is treated as a sharp boundary, whose motion is followed, i.e., the interface is identified with the control volume boundaries dividing the computational domain into more than one domain. For the second group, the interface is moved through a fixed grid and its position is computed at each time step and in all partially filled cells. The fixed-grid methods have the advantage of handling strong topological deformations of the interface such as merging and fragmentation, but it may fail to calculate the surface tension force accurately under certain circumstances. One of the

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Eulerian method in tracing the surface is volume-of-fluid method [1-7]. The VOF method solves a non-diffusive solution of the advection equation, by a geometrically based calculation technique of the void fraction fluxes at the cell faces based on the reconstructed interface. A significant improvement of the interface representation was achieved by Youngs [3] by introducing a piecewise-linear method (PLIC). The PLIC method approximate the interface is by a straight line of arbitrary orientation in each cell. Its orientation is found the distribution of one of the fluids in the neighbor cell. In this work the VOF-PLIC method has been used for tracking surface and exerting the effect of surface tension.

II. PROBLEM FORMULATION

The governing equations with considering the incompressibility of each fluid and without phase change across the interface are as follows:

$$\frac{\partial u_i}{\partial x_i} = 0 , \tag{1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \mathbf{F_v^{st}} \cdot \vec{i} + \mu \frac{\partial^2 u_i}{\partial x_j^2} + \rho g_i . \tag{2}$$

where u_i's are the velocity components, and t and x_i are time and space coordinates respectively, p is the pressure, $\vec{i}$ is the unit vector in the ith direction, $\mathbf{F_v^{st}}$ is the surface tension force per unit volume and ρ and μ are the average density and absolute viscosity in a cell, respectively and they depend on the densities and viscosities of each fluid a the cell. A volume-of-fluid (VOF) method along with a piecewise linear interface calculation is used to capture the fluid interfaces. That is:

$$\frac{\partial F}{\partial t} + u_i \frac{\partial F}{\partial x_i} = 0 \tag{3}$$

here, F is the volume fraction of fluid, which is F=1 in one fluid and F=0 in the other one, ρ and μ are density and viscosity of fluids, respectively, which can be defined by the function of volume fraction, density and viscosity in each fluid of the total extent as follows:

$$\rho = \rho_2 + F(\rho_1 - \rho_2) \quad \text{and} \quad \mu = \mu_2 + F(\mu_1 - \mu_2) \tag{4}$$

here, ρ and μ are density and viscosity of fluids, respectively and the subscripts 1 and 2 denote the two fluids involved.

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Here the Poisson equation is obtained by taking the divergence of the momentum equation and also the continuity equation, as follows:

$$\frac{\partial}{\partial x_i}(\frac{\partial p}{\partial x_i}) = -\frac{\partial}{\partial x_i}\left[\frac{\partial}{\partial x_j}(\rho u_i u_j - 2\mu S_{ij} - \frac{\mathbf{F_v^{st}} \cdot \vec{\mathbf{i}}}{\rho})\right]. \tag{5}$$

III. SURFACE TENSION FORCE

The complexity of simulation of interfacial flows is mainly due to the existence of surface tension force. The surface tension force is presented at the interface of two fluids when at least one of them is liquid. The surface tension force may be important in some interfacial flows. The surface tension force produces pressure jump across the interface. The boundary condition at the interface is stated as [8]:

$$(p_1 - p_2 + \sigma\kappa)n_i = (\tau_{1ik} - \tau_{2ik})n_k + \frac{\partial \sigma}{\partial x_i} \tag{6}$$

In this equation σ is surface tension coefficient, p_α is pressure, α denotes each of fluids and is defined as $\alpha=1,2$, $\tau_{\alpha ik}$ is viscous tension tensor, $\mathbf{n}$ is unit vector perpendicular to the surface (toward fluid 2) and κ denotes the interface curvature which is defined as follows:

$$\kappa = \frac{1}{R_1} + \frac{1}{R_2} \tag{7}$$

In this equation R_1 and R_2 are interface curvature radii in the principle axis.

If Eq. (6) is projected normal to the surface, the boundary condition for pressure is:

$$p_1 - p_2 + \sigma\kappa = 2\mu_1 n_k (\frac{\partial u_k}{\partial n})_1 - 2\mu_2 n_k (\frac{\partial u_k}{\partial n})_2 \tag{8}$$

From Eulerian point of view, surface tension force generates discontinuity in the pressure field. The discontinuity makes the numerical simulation of the interfacial flows difficult. There has been some efforts for implementing the effect of surface tension in Eulerian schemes. To eliminate the problem, the surface tension force is tuned into a volume force.

One of attempts in this field, were done by Brackbill *et al*. [9]. This method, which is called CSF method, effect surface tension is replaced to a volume force in the surface vicinity.

$$\vec{\mathbf{F}}_v^{st} = \sigma\kappa\delta_s \mathbf{n} \tag{9}$$

Where δ_s is the Dirac delta function, and $\mathbf{n}$ is the vector perpendicular to the face. This body force is added into the momentum equations and so the effect of surface tension is modeled. In this model it is necessary to calculate κ, n and δ_s. These variants are related to volume fraction function. By definition, they are calculated as follow [10]:

$$\mathbf{n} = \frac{\nabla \widetilde{F}}{|\nabla \widetilde{F}|} \quad , \quad \delta_s = |\nabla \widetilde{F}| \quad \text{and} \quad \kappa = -\nabla \cdot n \tag{10}$$

Since F is not a smooth function in VOF method, for calculating the parameters in Equations (10), firstly, the F function is averaged in order to obtain a smooth function, then derive it, which itself causes developing force $\mathbf{F_v^{st}}$ in neighboring interface [10]. Although the two fluids have high density difference, this causes the lighter fluid in the neighboring cells to accelerate and produce spurious currents, because the density correction term is added to reduce the force in the region with lighter fluid in momentum equation, due to the lightness of the fluid, it starts spurious movement. The characteristic of numerical methods is the susceptibility to the volume fraction smoothness (F) in the neighboring face, which model the surface tension; so that, for avoiding the strong spurious flows, it is necessary F smoothes in the adjacent surface. The amount of spurious velocity along with the accuracy of the pressure jump across the interface are use to evaluate the models. For CSF model, Eq. (9) is corrected to decrease the intensity of spurious currents by applying a density correction term [9, 10]:

$$\mathbf{F}_v^{st} = \sigma\kappa\boldsymbol{\delta_s}\mathbf{n} = \sigma\kappa\mathbf{n}|\nabla\widetilde{F}|\frac{\rho(x)}{[\rho]}, \tag{11}$$

This term is not obtained from any conversation law, but it is only postulated. Another model was presented by Lafaurie et al. [11] in 1994, is called CSS model. The CSS model, converts the surface tension force into stress form T, which is tangential to the interface and is given by:

$$\mathbf{T} = -\sigma(|\nabla F|\mathbf{I} - \frac{\nabla F \otimes \nabla F}{|\nabla F|}), \tag{12}$$

where $\otimes$ is the tensor product and I is the Kronecker tensor. In this method $\mathbf{F}_v^{st}$ is written as:

$$\mathbf{F}_v^{st} = -\nabla \cdot T = \sigma\nabla \cdot (|\nabla F|\mathbf{I} - \frac{\nabla F \otimes \nabla F}{|\nabla F|}), \tag{13}$$

Meier et *al*. [12] modeled surface tension force based on VOF-PLIC method. In their model the surface tension force per unit area is determined in interfacial cells only and multiplied by interface area. But in the stagger grid numerical methods, when the volume force is divided into the momentum cells and fluid accelerates as result of the surface tension. Since they used a staggered-mesh layout, they portioned $e_{x,i,j}$ on the staggered momentum control volumes by means of some weighted averaging.

$$\mathbf{e_{x,i,j}} = \frac{\sigma}{\rho_{i,j}}\kappa_{i,j}\frac{A_{i,j}}{V_{i,g}}\mathbf{n_{i,j}} \tag{14}$$

Despite of their simplicity and being conservative, CSS and CSF models produce high spurious currents near the interface. These currents are strongly growing vertical flows in the interfacial and it neighboring cells. Meier's model was able to reduce spurious currents to some extent; however it still suffers from the generation of the spurious currents.

PCIL model was presented by Shirani et *al*. [13] to reduce the amounts of these currents in 2005. This model is based on VOF-PLIC in which surface tension force is obtained by

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modified CSS and CSF models by introducing a dimensionless parameter H. This parameter is the ratio of the cell face area occupied by heavier fluid to total cell face area.

$$\mathbf{F_v^{st}} = H\sigma\kappa\mathbf{n}\frac{\left|\nabla\tilde{F}\right|}{[F]} \quad \text{and} \quad \mathbf{F_v^{st}} = H\sigma\nabla\cdot\left(\left|\nabla F\right|\mathbf{I} - \frac{\nabla F \otimes \nabla F}{\left|\nabla F\right|}\right) \quad (15)$$

Seifollahi et al. [14] presented a new model called SGIP for surface tension force based on VOF-PLIC and directly calculated the surface tension force at each interfacial cells in 2007. They applied their model for two-dimensional droplets and bubbles. In this model, the surface tension force directly was calculated in momentum Equations.

IV. Generalized SGIP Model for Three-Dimensional Flows

Seifollahi and Shirani extend SGIP model for two-dimensional cases surface tension [14]. If the Equations are developed in three- dimensional cases, the surface tension force in each cell in one location is as follow:

$$F_{v\alpha,i,j,k}^{st} = \frac{\sigma\kappa_{i,j,k}A_{\alpha,i,j,k}}{V_{i,j,k}} \quad \text{and}$$

$$A_{x,i,j,k} = S_{x,i+1/2,j,k} - S_{x,i-1/2,j,k} \quad \text{and} \quad (16)$$

$$A_{y,i,j,k} = S_{y,i,j+1/2,k} - S_{y,i,j-1/2,k} \quad \text{and}$$

$$A_{z,i,j,k} = S_{z,i,j,k+1/2} - S_{z,i,j,k-1/2}$$

where $\alpha = 1, 2, 3$ represent the figures in three directions. The values of figured surface in x, y and z directions, regarding both the interface in each cell and the calculation of the values of "S" components are determined (Fig. 1).
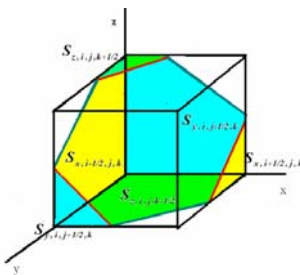

Fig. 1 An interfacial cell and some of the "S" components

The values of S_x, S_y and S_z are related to the location of interface in a cell and since we are using the PLIC technique, in cells i,j,k, the interface shape is a plane surface and its formulation is known. So the calculation of the values of $S_{x,i,j,k}$, $S_{y,i,j,k}$ and $S_{z,i,j,k}$ is straightforward and can be done with negligible computational cost. As shown in Fig. 2, there are eight possible cases where the interface shape is triangular, quadrilateral section A, quadrilateral section B, pentagonal section A, pentagonal section B, pentagonal section C, pentagonal section D and hexagonal section. Number of all possible cases are 27 but here, only eight cases when $n_x\geq0$, $n_y\geq0$, $n_z\geq0$ and $F<0.5$ are studied. Other cases can be

determined by mirror method regarding to above mentioned subjects. To simplify, it is supposed that the cell dimensions are unit. Regarding the amount of the vector which is perpendicular to the interface, its Eq. is calculated in each cell as follows:

$$n_1 x + n_2 y + n_3 z = d \quad (17)$$

in the Equation n_1, n_2 and n_3 are defined as:

$$n_1 = Min(\left|n_x\right|,\left|n_y\right|,\left|n_z\right|) \,, \quad n_3 = Max(\left|n_x\right|,\left|n_y\right|,\left|n_z\right|) \,\, and$$

$$n_2 = \left|n_x\right| + \left|n_y\right| + \left|n_z\right| - n_1 - n_3 \quad (18)$$

In the above Equation, , $n_{x,i,j,k}$, $n_{y,i,j,k}$ and $n_{z,i,j,k}$ are the values perpendicular to the interface in each cell (i, j, k), which are calculated in Eq. (10) by volume fraction function in cell (F).
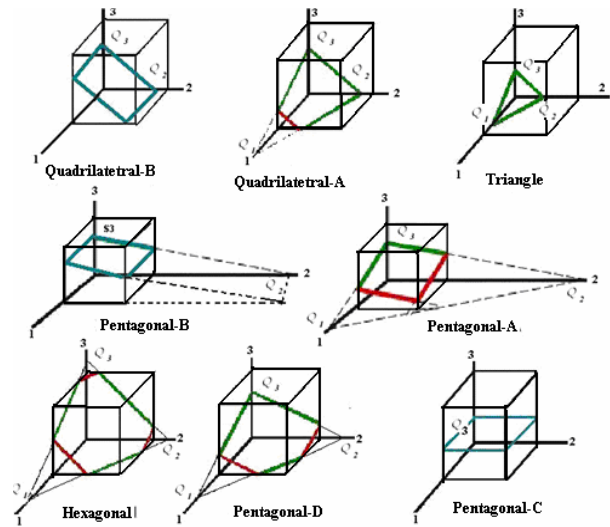

Fig. 2 Different configurations for an interface position of each cell for the 3D cases, when $n_x \geq 0$, $n_y \geq 0$, $n_z \geq 0$ and $F<0.5$

The vector m is defined as the gradient of the volume fraction function for a uniform numerical grid with unit length and is:

$$m_{x,i,j,k} = -(F_{i-1,j-1,k-1} + F_{i-1,j-1,k+1} + F_{i-1,j+1,k-1} + F_{i-1,j+1,k+1}$$
$$+ 2(F_{i-1,j-1,k} + F_{i-1,j+1,k} + F_{i-1,j,k-1} + F_{i-1,j,k+1}) + 4F_{i-1,j,k}) +$$
$$(F_{i+1,j-1,k-1} + F_{i+1,j-1,k+1} + F_{i+1,j+1,k-1} + F_{i+1,j+1,k+1} + 2(F_{i+1,j-1,k}$$
$$+ F_{i+1,j+1,k} + F_{i+1,j,k-1} + F_{i+1,j,k+1}) + 4F_{i+1,j,k}) \quad (19)$$

$$m_{y,i,j,k} = -(F_{i-1,j-1,k-1} + F_{i-1,j-1,k+1} + F_{i+1,j-1,k-1} + F_{i+1,j-1,k+1}$$
$$+ 2(F_{i-1,j-1,k} + F_{i+1,j-1,k} + F_{i,j-1,k-1} + F_{i,j-1,k+1}) + 4F_{i,j-1,k}) +$$
$$(F_{i-1,j+1,k-1} + F_{i-1,j+1,k+1} + F_{i+1,j+1,k-1} + F_{i+1,j+1,k+1} + 2(F_{i-1,j+1,k}$$
$$+ F_{i+1,j+1,k} + F_{i,j+1,k-1} + F_{i,j+1,k+1}) + 4F_{i,j+1,k}) \quad (20)$$

$$m_{z,i,j,k} = -(F_{i-1,j-1,k-1} + F_{i-1,j+1,k-1} + F_{i+1,j-1,k-1} + F_{i+1,j+1,k-1}$$
$$+ 2(F_{i-1,j,k-1} + F_{i+1,j,k-1} + F_{i,j-1,k-1} + F_{i,j+1,k-1}) + 4F_{i,j,k-1}) +$$
$$(F_{i-1,j-1,k+1} + F_{i-1,j+1,k+1} + F_{i+1,j-1,k+1} + F_{i+1,j+1,k+1} + 2(F_{i-1,j,k+1}$$
$$+ F_{i+1,j,k+1} + F_{i,j-1,k+1} + F_{i,j+1,k+1}) + 4F_{i,j,k+1}) \quad (21)$$

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Thus with having **m** vector and according to Eq. (10), the components of the vector perpendicular to the interface will be:

$$n_{x,i,j,k} = -\frac{m_{x,i,j,k}}{\sqrt{m_{x,i,j,k}^2 + m_{y,i,j,k}^2 + m_{z,i,j,k}^2}} \quad (22)$$

$$n_{y,i,j,k} = -\frac{m_{y,i,j,k}}{\sqrt{m_{x,i,j,k}^2 + m_{y,i,j,k}^2 + m_{z,i,j,k}^2}} \quad (23)$$

$$n_{z,i,j,k} = -\frac{m_{z,i,j,k}}{\sqrt{m_{x,i,j,k}^2 + m_{y,i,j,k}^2 + m_{z,i,j,k}^2}} \quad (24)$$

These are components of **n** along the x_1, x_2 and x_3 axes (note that x_1, x_2 and x_3 axes are not necessarily the same as x, y, and z axes). Let d denotes the distance of origin from the plane interface. The intercepts of this plane on the x_1, x_2 and x_3 axes are:

$$Q_1 = \frac{d}{n_1} \quad , \quad Q_2 = \frac{d}{n_2} \quad , \quad Q_3 = \frac{d}{n_3} \quad (25)$$

In order to match the volume fraction, we need to find the value of d for which the volume of the cubic cell beneath the plane is equal to F. Here, it is assumed that the cell dimensions are unit for simplicity. As shown in Fig. 2, there are eight possible cases where the interface shape is triangular, quadrilateral section A, quadrilateral section B, pentagonal section A, pentagonal section B, pentagonal section C, pentagonal section D and hexagonal section. Number of all possible cases are 27. Other cases can be determined by mirror method regarding to above mentioned subjects. For triangular section using the dimensions Q_1, Q_2 and Q_3, we have:

$$\cancel{V} = \frac{d^3}{6n_1 n_2 n_3} \quad (26)$$

where $\cancel{V}$ is the volume of triangle section. The volume of the part of the cell beneath the plane (triangular section for this case) is equal to F. Thus, for triangular section case, the value of d is determined as:

$$d = \sqrt[3]{6Fn_1 n_2 n_3} \quad (27)$$

For triangular section, all the value Q_1, Q_2 and Q_3 are less than 1. Note that in some cases (quadrilateral, pentagonal and hexagonal section), Q_1, Q_2 and Q_3 exceed 1. For triangular case, we have:

$$0 \leq Q_3 \leq Q_2 \leq Q_1 \leq 1 \quad \text{and} \quad 6F n_1 n_2 n_3 \leq n_1^3 \quad (28)$$

The value of the interface area in the cell is calculated as:

$$A = 0.5\sqrt{(Q_1 Q_3)^2 + (Q_2 Q_3)^2 + (Q_1 Q_2)^2} \quad (29)$$

The cases of quadrilateral, pentagonal or hexagonal section cases in calculating grid cell may be obtained similarly. After calculating the interface area for a uniform numerical grid with unit length, the projections of the interface area in the x, y and z directions can be calculated. For uniform grid of length h, we have:

$$A_{x,i,j,k} = A_{i,j,k} h^2 n_x \; , \; A_{y,i,j,k} = A_{i,j,k} h^2 n_y \; , \; A_{z,i,j,k} = A_{i,j,k} h^2 n_z \quad (30)$$

V. NUMERICAL METHOD

A three-dimensional computer research code is modified and used to simulate the flow. The code is finite volume based and uses SIMPLEC algorithm along with QUICK method for convective terms. The code has the ability to solve laminar and turbulent, steady and unsteady flows. The code which was originally set up for solving single fluid flows was modified to solve interfacial flows. The VOF_PLIC method was used for interface tracking and the SGIP, CSF, CSS and PCIL models were implemented into the code.

VI. RESULTS

To show the performance of three-dimensional model of SGIP, motionless drop of liquid and bubble of gas in a surrounding fluid with different density and viscosity are studied. Physically, in the absence of the gravity, the droplet or the bubble should remain motionless and pressure jump as a result of surface tension force must obey Eq. (8). Assuming σ to be constant, the Eq. (8) is simplified to:

$$p_1 - p_2 = \sigma\kappa . \quad (31)$$

where, $\kappa = 2/R$ is the surface curvature of the drop or bubble and R denotes the drop or bubble radius. Although, physically the droplet or bubble should be stationary, some spurious currents are produced numerically due to the modeling of surface tension force. The spurious currents may cause interface deformation and the pressure jump may be differed from that of its physical value. To consider static drop and static bubble, we used water, ρ_1=1000 kg/m3 and μ_1= 0.001 N.s/m2, and air, ρ_2 =1.2 kg/m3 and μ_2 = 1.8e-5 N.s/m2. The surface tension coefficient is σ = 0.073 N/m; here 1 is for drop and bubble and 2 is for flows around them. We chose the number of grid points to be 64×64×64 for the computational regions and the time step is kept constant. The spherical drop or bubble with the radius 0.016 m is located at the center of a cubic box. Time step has been chosen 0.01s.

Static Drop

To show the ability of the SGIP model for three-dimensional flows in comparison with other models, pressure contours, maximum spurious velocities, norm spurious flow velocities and pressure jump error are calculated using different models. The norm of the spurious currents is defined as the average of the absolute velocity in the flow field. Figs. 3 and 4 show the variation of maximum and norm of spurious velocities with time using different models. As it is seen from Figs. 3 and 4, the CSF model generates higher maximum and second order of norm spurious velocities. Adding PCIL model or density correction condition to CSF model, the magnitude of spurious velocities is reduced to some extent. The maximum and second order norm of spurious velocities for

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CSS model have lower values in compare with the results obtained for CSF model. Spurious currents are somewhat reduced by adding PCIL model to CSS model.
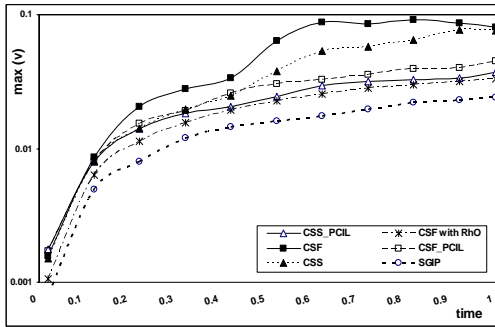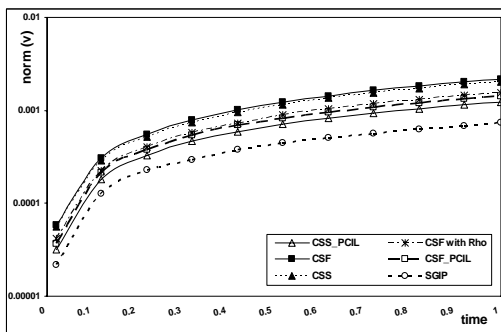

Fig. 3 Maximum spurious velocities for drop

Fig. 4 Norm spurious velocities for drop

Figs. 3 and 4 show the fact that maximum and second order norm spurious velocities created in SGIP model have the lowest values among the other models. Figs. 5 and 6 show the pressure contours and pressure jump relative errors for static drop using all six different models, respectively. As it is observed pressure has some oscillations near the interface. It is seen that the pressure contour of SGIP model is smoother than other models and it also produces more accurate values for pressure.
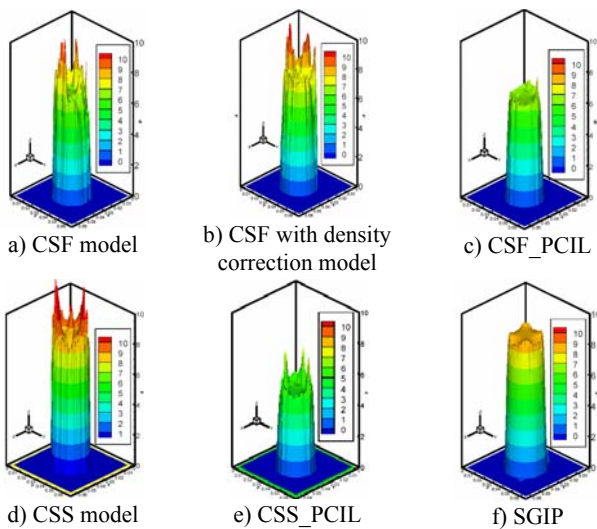

a) CSF model
b) CSF with density correction model
c) CSF_PCIL
d) CSS model
e) CSS_PCIL
f) SGIP

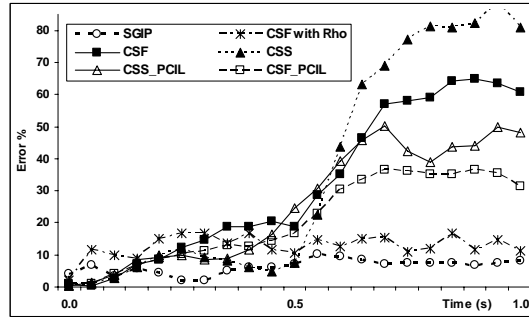Fig. 5 Pressure contour lines for a 3D drop

Fig. 6 Time evolution of error for pressure jump across the interface of a static drop

Static Bubble

To insure the high performance of the SGIP model for three-dimensional flows, we also simulated the flows for the interface curvature being toward the lighter fluid (concave surface). For this purpose, the static bubble of air surrounded by water has been studied. Physically, it is expected that the initial state in the absence of the gravity force is maintained and no spurious current should be produced. But as mentioned before, due to the modeling of surface tension force, the numerical simulation produces spurious currents. These currents can cause interface deformation and the pressure jump deviates from its exact value. Figs. 7 and 8 show the variation of maximum and norm of spurious velocities with time using different models respectively.
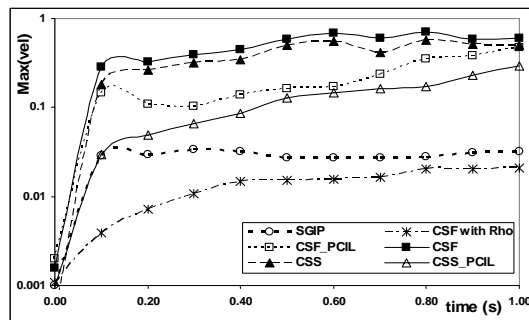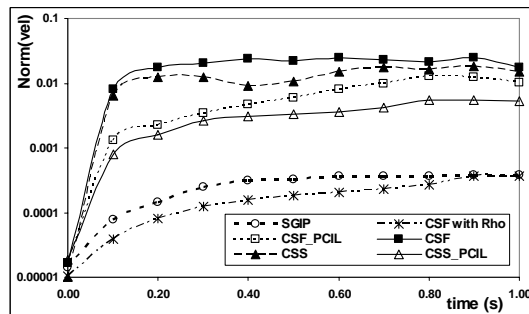

Fig. 7 Maximum spurious velocities for bubble

Fig. 8 Norm spurious velocities for bubble

As it is seen from the figures, the CSF model generates higher maximum and second order norm of spurious velocities. By adding PCIL or density correction condition to

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CSF model, spurious currents are reduced. The maximum and second order norm of spurious velocities generated with SGIP model is lower than that of the other models expect the CSF model with the density correction. But as we see in the next figures, CSF model with the density correction reduces the spurious currents at the expense of the incorrect pressure jump. Fig. 9 shows the value of pressure jump relative error for three-dimensional bubble after one second using different models. The largest error is obtained by CSF model with the density correction, it is 75 percent after one second, while for SGIP models, the maximum error is only 8.8 percent.
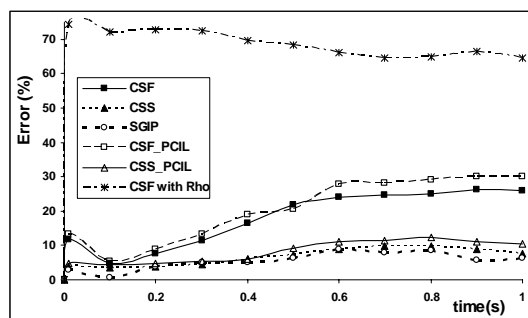

Fig. 9 Time evolution of *error* for the pressure jump across the interface of a static bubble

VII. CONCLUSION

In this paper, six different surface tension models for interfacial flows were studied and compared for static case. The performance of each model was examined by calculating the spurious currents and pressure jump error for static drop and bubble. The pressure contours and the maximum and norm spurious velocities for the three-dimensional static bubble and drop produced by different surface tension models presented. It was shown that the SGIP model which was generalized for three-dimensional cases is much more accurate than the other models.

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